

5050-0031  
PATENT

The output preferably further comprises a list of the genes that are modulated (up-regulated or down-regulated) in the test gene expression profile, as compared with a pre-established expression value, a pre-selected standard expression profile, a second test gene expression profile, or another pre-set threshold value.

- 5 The output is preferably hyperlinked, so that the operator can easily switch from, for example, a listing of the similar standard expression profiles to a listing of the modulated genes in a selected standard expression profile, or from a gene listed in the test profile to a list of the standard expression profiles in which the gene is similarly modulated, or to a list of the standard compounds (and/or conditions) which appear to modulate the selected gene. The output can comprise correlation information that highlights features in common between different genes, targets, profiles, compounds, assays, and the like, to assist the user in drawing useful correlations. For example, the output can contain a list of genes that were modulated in the user's experiment with a selected compound: if a plurality of the genes are indicated as associated with liver toxicity, the system can prompt the user that the compound is associated with a toxic drug signature, and prompt the user to continue with the next compound. Conversely, the output could indicate previously unnoticed associations between different pathways, leading the user to explore a hitherto unknown connection. The output preferably includes hyperlinks to product information, encouraging the user to purchase or order one or more products from a selected vendor, where the product(s) relate specifically to the focus of the database inquiry and the correlation information that results, and is presented back to the user to facilitate hypothesis generation. For example, the output can provide links to products useful for confirming the apparent activity of a compound, for measuring biological activity directly, for assaying the compound for possible side effects, and the like, prompting the user to select products useful in the next stage of experimentation.

- The system is preferably provided with an algorithm for assessing similarity of compounds. Suitable methods for comparing compounds and determining their morphological similarity include "3D-MI", as set forth in copending application USSN 09/475413, <sup>now US Pat 6,470,305,</sup> incorporated herein by reference in full, Tanimoto similarity (Daylight Software), and the like. Preferably, the system can be queried for any compounds that are similar to the test compound in structure and/or morphology. The output from this query

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